



CENTRE FOR DOCTORAL TRAINING

**Email**: sushy@nottingham.ac.uk **Website**: www.sustainablehydrogen-cdt.ac.uk

## Annual Report 2023















Engineering and Physical Sciences Research Council



## Sustainable Hydrogen Centre for Doctoral Training (SusHy CDT) established 2019.

The Centre is the first UK hydrogen energy CDT, selected through the £446 million CDT call from the Engineering and Physical Sciences Research Council (EPSRC) aimed at tackling pressing global challenges.SusHy CDT has **four** partner universities – **Nottingham, Loughborough, Birmingham and Ulster** – and **four** overarching Centre objectives (see **Vision** below).

We have recruited a total of 65 talented individuals to our CDT, which is providing high quality, multi-disciplinary training to achieve mass uptake of hydrogen technologies in the UK and beyond. As of October 2023, having recruited five cohorts of students, they work on hydrogen combustion, distribution, production, safety, storage, systems and upgrade. The CDT is supported by the EPSRC and over 40 Stakeholder partners.



## **Our Vision**

In-line with the UK's commitment to reduce emissions by **78% by 2035** and achieve **Net Zero by 2050**, we're developing hydrogen technologies facilitating deep-decarbonisation.

#### Sustainable Hydrogen CDT's objectives:

- Deliver high quality trans-disciplinary training covering fundamental science, applied engineering, and systems issues and build an appreciation of societal barriers to innovation.
- Through innovation opportunities, build initiative and stimulate an entrepreneurial mindset.
- Deliver 'industry ready' doctorates, who have a comprehensive skill set and experiences.
- Co-create research ideas and undertake, in partnership with our stakeholders, cutting edge investigations of hydrogen-based solutions to deep decarbonisation of the energy system.



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### **Executive Summary**

This year is the final recruitment year for the SusHy CDT and we have welcomed 19 new students as of October 2023 across our four partner universities from an overwhelming 456 total applications. The SusHy CDT commitment to recruiting diverse teams has been very successful, encouraging applications from a wide social cross-section; with our advertising giving candidates from under-represented groups the confidence to apply. This has been accomplished without compromising on academic excellence, as the highly talented set of individuals in Cohort 5 show.

As of October 2023, our latest Cohort has 58% of students identifying as from ethnic minority communities and 32% of students identifying as female. The former statistic improves significantly on previous years, and students from ethnic minority communities now make up 41% across all cohorts as recruited. Whilst the latter is much higher than the UK STEM sector's, where only around 24% of the workforce are female. 16% of all our students identify as being part of the LGBTQ+ community, and examples of the SusHy CDT's efforts to create a supportive and inclusive environment for students can be found in this Report.

The SusHy CDT acquired 2 additional stakeholders and partners this year, National Gas, and the National Nuclear Laboratory. We are excited to see how these relationships develop further in 2024. We ran a stakeholder challenge event in February 2023 which was set by Romco Metals in collaboration with The Community Revolution CIC where the CDT students came up with less polluting fuel solutions to run the furnaces at its Ghana facility, currently oil-powered. A stakeholder event was held at the University of Nottingham in April 2023, looking at routes (and potential barriers) to the greater use of hydrogen power in our communities, particularly rural ones. The speakers included Neil (Ming-En) Han from Nottingham City Council, Tony Gray from Rutland Community Ventures CLG and Matt Barney from GeoPura.

In June 2023, a group of SusHy students (Get With The H2ype) ran a Hydrogen stall and activity centre at the Glastonbury Festival's Science Futures Field to bring hydrogen education to the general public, engaging with over 1,000 festival-goers. The SusHy CDT organised a joint Power Trader Game workshop at Cardiff University for Cohorts 3 and 4 students, in collaboration with the Resilient Decarbonised Fuel Energy Systems CDT. This also included a visit to Cardiff's Gas Turbine Research Centre.

The annual SusHy CDT Conference was held in July 2023 in Loughborough and included a thought–provoking talk in green hydrogen via electrolysis from Prof. Amitava Roy, CEO of Engas Global and visiting professor at Loughborough University, oral and poster presentations by SusHy students and cohort building activities. The SusHy CDT organised a visit to the National Space Centre for the students as part of this year's away day activity.

SusHy students presented their research at various events and conferences including the 2022 Early Career Researcher Regional Symposium on Electrochemistry, the 17th International Symposium on Metal-Hydrogen Systems (MH2022), 'The Future of Green Energy' webinar, the 2nd H2FC International Summer School, the 10th International Conference on Hydrogen Safety and the 14th International Solvothermal and Hydrothermal Association conference. Further examples of what staff and students have been up to this year can be found in pages 10 and 11 in the report.

As we reflect on our achievements, we'd like to thank all of our students, stakeholders, and partners for a truly excellent year in the SusHy CDT. We look forward to another year of SusHy CDT events.



### Equality, Diversity and Inclusivity (EDI)

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#### We recruit amazing individuals from a diverse talent pool

- SusHy CDT knows teams reflecting societal diversity are more successful, which is why we've put EDI at the heart of our operations. Our social media recruitment posts reflect CDT gender and cultural diversity, and back relevant advocacy dates, including but not limited to LGBTQ+ History Month in February, Pride Month in June, International Women in Engineering Day on June 23rd, and Black History Month in October.
- Our revised Recruitment Strategy is working; showing increased interest from female applicants, with **32%** of applicants identifying as female in 2022/23, increased from **29%** of applicants in 2021/22.
- Following our latest recruitment cycle, **16%** of all CDT students identify as part of the LGBTQ+ community.
- Interview procedures have been altered to better take into account students' different neurodiversity needs.

The CDT's programme aims to train the energy leaders we need to meet the Net Zero global challenge, which will require leading successful innovation teams informed by diverse perspectives.

#### We create a more inclusive environment with:

- Our **Student EDI Forum** and the **EDI Student Representatives** at Management Board meetings, give students direct influence on CDT EDI policy and opportunities to deal with issues.
- The '**Buddy Scheme**', an idea from CDT student Mickella Dawkins, matches current with new intake students, to ease any stresses around beginning a PhD and address concerns.
- The **EDI** Access Fund financially assists students if they have disability, mobility or domestic (child care) needs, which might otherwise prevent participation in activities.
- In July 2023, former CDT Director Prof. Gavin Walker, talked about where EDI impacts through the life of a project and how to incorporate EDI into a proposal, touching on the EDI plan he did for the SusHy CDT as an example for discussion during the EDI workshop at University of Nottingham.
- The CDT is a proud partner of the **Women's Engineering Society** (WES) and **Women Into Science and Engineering** (WISE), and provides free membership for students.



#### Examples of cohort diversity are reflected in following:

We seek to provide and continuously improve our supportive environment, where everyone feels equally valued and able to achieve their full potential. Recruitment aims are for a student community reflecting UK diversity; including LGBTQ+, disability, neurodiversity and socio-economic background. Among the diversity figures we pay close attention to are:

Ethnic Minorities	Gender parity	
<b>58%</b> of Cohort 5 identify as part of Ethnic Minority community	<b>32%</b> of Cohort 5 identify as female	
Across ALL CDT Cohorts (1-5) these students now account for	Across ALL CDT Cohorts (1-5) these students now account for	
41%	33%	
of all students (as of Oct 2023)	of all students (as of Oct 2023)	

## SusHy CDT Team



Gavin Walker, CDT Director until September 2023

### Sanliang Ling, CDT Director since September 2023

sanliang.ling@nottingham.ac.uk



Kandavel Manickam, Programme Manager until April 2023





Gulcan Serdaroglu, Programme Manager since May 2023

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Sean Kirby, Marketing Manager until June 2023

Ella Crowther, Marketing Officer since July 2023

ella.crowther@nottingham.ac.uk



Esther Little, Administrative Officer

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## SusHy CDT Management Board







Associate Professor Sanliang Ling Director: SusHy CDT



Professor **Deborah Kays** Co-Director: EDI Support





Ulster University



Professor **Dani Strickland** Co-Director: **EDI Support** 

Professor

**David Saal** 

**Co-Director** 



Professor **David Book** Co-Director



**Dr Daniel Reed** Co-Director: Student Engagement



**Dr Dmitriy** Makarov **Co-Director** 

Professor

Vladimir

Molkov

**Co-Director** 



Professor Monica Guiletti **Co-Director** (until Sept 23)



Professor Wen-Feng Lin **Co-Director** (since Sept 23)







Dr Rafael Orozco **Co-Director** 



Professor Upul Wijayantha Co-Director: **EDI Support** (previously at Loughborough, now Cranfield)



### **Our Students**



### **Stakeholders**

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We work with 40-plus partners and stakeholders including energy providers, researchers, UK government and engineering consultancies. Such links are vital as the CDT pursues its four overarching objectives; particularly, delivering 'industry ready' doctorates and cocreating research ideas in collaboration with stakeholders. A Stakeholder list is at: www.sustainablehydrogen-cdt.ac.uk/stakeholders/stakeholders.aspx

#### **Stakeholders Supporting PhD Projects:**

Sustainable Hydrogen CDT gratefully acknowledges those stakeholders collaborating on students' PhD projects, ensuring our research is answering those guestions the hydrogen sector needs to further develop. ROLLS



Regular CDT Stakeholder Events enable students to network, and in Stakeholder Challenges partners give students real sector issues to work on.

#### February 2023 Stakeholder Challenge

This SusHy CDT Stakeholder Challenge was set by Romco Metals, a multi-national, non-ferrous metals recycler operating in Nigeria and Ghana and The Community Revolution CIC, a Nottingham-based renewable energy social enterprise, looking to enter the renewable energy business in Africa. The students were challenged to come up with less polluting solutions as an alternative to oil-powered furnaces considering issues such as the practicality of installing 'greener' technologies, available expertise and reliability.

#### April 2023 Stakeholder Workshop at UoN

This stakeholder event focussed on 'Hydrogen Communities'; discussing the opportunities, benefits and barriers for the use of hydrogen in energy communities and included an interactive workshop on exploring these issues for rural communities. Speakers included:

- Neil (Ming-En) Han Senior Energy Projects • Officer, Midlands Net Zero Hub
- Tony Gray Director of Rutland Community • Ventures CLG
- Matt Barney, Business Development Manager, . GeoPura.





## SusHy CDT News and Events 2022-2023

### October

The SusHy CDT welcomed its fourth Cohort of 11 students. Induction Week featured 'getting to know you' events, training sessions, research facility visits; and lunch and dinner dates, and some bowling, to give new students the chance to meet other students, and CDT staff and supervisors.



November-

SusHy CDT staff and students attended the 17th International Symposium on Metal-Hydrogen Systems (or MH2022) in Perth, Australia. At MH2022 Prof Gavin Walker was also selected as Chair of the MH International Steering Committee.

> Courtney Quinn, University of Nottingham, presented her work on Non-Stoichiometric Protic Ionic Liquid Electrolytes at the 2022 Early Career Researcher Regional Symposium on

Electrochemistry, at Queen's University Belfast.

### December January

The SusHy CDT Director, Prof Gavin Walker, was a key speaker at the 2022 Midlands Energy Summit.



A good time was had by CDT students at the SusHy CDT Winter Event gettogether, held in Birmingham including visit to the city's Christmas Market, CDT meal and karaoke singing.



CDT students co-hosted and presented at a webinar on 'The Future of Green Energy', run by Climate LinkUp. Kieran Heeley (University of Birmingham) and Courtney Quinn (University of Nottingham) were event co-hosts and Srinivas Sivaraman (Ulster University) spoke on: Ammonia as a promising hydrogen carrier and clean fuel.

February

March

Aryamman Sanyal (Loughborough University) attended the 2023 Hydrogen and Fuel Cells Conference with a theme of 'Fuelling the Future Now'.



The SusHy CDT Stakeholder Challenge, set by Romco Metals in collaboration with The Community Revolution CIC, had CDT students come up with a less polluting fuel to run the furnaces at its Ghana facility, currently oilpowered.

## SusHy CDT News and Events 2022-2023



A Stakeholder Event was held at University of Nottingham, looking at routes (and potential barriers) to the greater use of hydrogen power in our communities, particularly rural ones. The International Energy Agency's latest Hydrogen Technology Collaboration Programme workshop was held at SusHy CDT's Nottingham base. Prof Gavin Walker, CDT Director, was one of around 30 delegates from across the world attending the event, to help shape a secure and sustainable energy sector for the future.

May





A group of SusHy students (Get With The H2ype) ran a Hydrogen stall and activity centre at the Glastonbury Festival's Science Futures Field to bring hydrogen education to the general public, engaging with over 1000 festival-goers.



### July

August

The annual SusHy CDT Conference was held 18-19th July in Loughborough, and included oral and poster presentations by CDT cohorts.

This year's CDT awayday was at the National Space Centre in Leicester, which included watching an awardwinning show in the UK's largest planetarium.



SusHy CDT students took part in a joint Power Trader Game workshop at Cardiff University, co-organised with the Resilient Decarbonised Fuel Energy Systems CDT.

### September

Ulster University SusHy Students Mina Kazemi, Hazhir Ebne Abbasi and Srinivas Sivaraman presented their research at the 2nd H2FC Summer School held at University of Porto, Portugal.

> Ulster University SusHy students Mina Kazemi, Hazhir Ebne Abbasi and Srinivas Sivaraman presented their latest research findings at 10th International Conference on Hydrogen Safety in Quebec City.

Kieran Heeley (University of Birmingham) presented his research at the 14th bi-annual International Solvothermal and Hydrothermal Association (ISHA) conference in Valladolid, Spain.



Courtney Quinn, co-hosted the 'Nature Positive Solutions for Climate Resilience' webinar for Climate LinkUp.

### **Current Research**

Our Sustainable Hydrogen CDT PhD students, across all five Cohorts, are undertaking hydrogen research in a wide variety of areas.

In this section you will find research profiles for each CDT student researcher; working in areas such as Combustion, Distribution, Production, Safety, Storage, Systems, and Upgrade.

Vehicle

and end-of-life management





Life cycle greenhouse gas emissions **Circular resource management** Competitiveness with other low carbon options **UK policy and fleet-level implications** 







Antonia Dase (Cohort 2) **School of Chemistry** 



#### Development of dehydrogenation catalysts for hydrogen storage materials

Antonia is working on the development of catalysts based upon earth abundant metals for application towards hydrogen storage materials including ammonia borane and metal borohydride ammoniates. Critical to the project is developing a fundamental understanding of the mechanisms involved the dehydrogenation of these materials in order to optimise catalytic performance.

Supervisors: Professor Deborah Kays, Dr Saad Salman, Professor David Grant





Ulster University

Hazhir Ebne-Abbasi (Cohort 2) Belfast School of Architecture and the Built Environment (BSABE)



Figure 1. CFD modelling of a sub-cooled liquid hydrogen station

#### CFD model of fuelling through the entire equipment of a hydrogen refuelling station

Since joining HySAFER (Hydrogen Safety Engineering and Research) at Ulster University Hazhir has contributed to a number of projects, including HyTunnel-CS, and SH2APED. He is now focusing on the development and validation of the first of its type CFD model for simulation of complex heat and mass transfer processes during refuelling; through the entire chain of equipment at HRS from a high-pressure tank through piping, pressure control valve, precooler, breakaway, hose, nozzle, etc. to onboard storage tanks. The research would be followed by focus on modelling sub-cooled liquid hydrogen stations.

Supervisors: Dr Dmitriy Makarov, Professor Vladimir Molkov.





Bakhtawar Ahmed (Cohort 4) School of Chemistry



#### Developing imide/amide catalysts for the ammonia decomposition process to produce hydrogen

Ammonia has the potential to provide itself as an effective medium for energy storage in the form of hydrogen. Implementing this idea of transforming existing hydrocarbon-based energy sources to renewable and essentially zero carbon energy in the form of hydrogen, requires overcoming limitations and working on research gaps.

The production of hydrogen from ammonia (NH ) through catalytic decomposition has gained significant attention as a potential avenue for clean and efficient hydrogen production. Developing efficient catalysts for this process is crucial to enhance the kinetics and selectivity of ammonia decomposition, thereby enabling the large-scale utilization of ammonia as a hydrogen carrier. Bakhtawar's project will explore group 2 and transition metal imide/amide catalysts for ammonia decomposition, with an aim to operate the process at lower temperature and pressure. Bakhtawar will investigate sustainable catalysts, avoiding resource limited rare earth metals.

Supervisor: Associate Professor Joshua Makepeace



Stakeholder collaboration





#### Ben Drake (Cohort 5) Faculty of Engineering





#### Investigating the use of alternative fuel pump designs for cleaner aviation

Civil aviation needs to transition from kerosene to more sustainable fuels, liquid hydrogen (LH2) has emerged as a promising candidate. One key technological barrier to LH2 fuelled flight is reliably pumping the cryogen to the jet engines at sufficient rates for the duration of the pump's life cycle. LH2 turbopumps have existed for decades in the rocketry sector but with an active service life measured only in minutes and not the 10,000+ hours required for civil aviation. The lifespan of a LH2 turbopump is dictated by the failure of its bearing components, a consequence of traditional lubrication being unviable in cryogenic temperatures.

Ben will explore the operation of bearings in the harsh conditions by modelling various candidates, including foil, electromagnetic, and more conventional fluid bearing designs. The research will also explore the potential use of solid lubricants to further reduce wear.

Supervisors: Dr Benjamin Rothwell, Dr Mohammadreza Amoozgar, Professor Seamus Garvey, Dr Rajab Omar



#### Stakeholder collaboration



#### Quantifying environmental and resource impacts of the future UK hydrogen-fuelled vehicle fleet

Cheryl's project is developing novel Life Cycle Assessment (LCA) models to assess the resource and environmental implications of deploying hydrogenfuelled vehicles in the UK's light duty and heavy duty road fleets. Cheryl's comprehensive approach will consider the current and future mix of hydrogen production routes, vehicle manufacture and use, and end-of-life vehicle management (e.g. recycling).

Beyond more common LCA studies comparing technologies on a vehicular level, this project will consider the turnover of UK vehicle fleet and the uptake of hydrogen technologies, to quantify cumulative resource and environmental implications.

Supervisor: Professor Jon McKechnie







Esther Mgbemeje (Cohort 5) Department of Chemical Engineering



#### Green hydrogen production from water splitting powered by renewable electricity

Esther's research will build upon recent fundamental research on new electrocatalysts and electrodes for water electrolysis, and the anion-exchangemembrane (AEM) to further develop membrane-electrode-assembly based water electrolyser for sustainable hydrogen production with the maximum resource and energy efficiencies. Particular attention will be paid to the catalytic electrode-electrolyte interface structure to achieve efficient reaction kinetic, and fast charge and mass transports in the water electrolyser, to minimise overpotential loss and gain maximum voltage and overall system efficiency. The life cycle assessment will also be considered at component levels.

Supervisors: Professor Wen-Feng Lin, Dr Simon Kondrat





Amy Liscoe (Cohort 5) School of Psychology



#### Public values for a hydrogen energy system

Amy's project will investigate the public's view of novel sustainable technologies and their willingness to engage with a hydrogen fuelled future. Overcoming barriers to acceptance and investigating methods of increasing engagement are imperative elements of Amy's research. By appreciating the perspectives and views of individuals from all backgrounds, industries, and ways of life Amy aims to initiate an area of research which can progress the acceptance and application of hydrogen technologies in our society.

Supervisors: Associate Professor Alexa Spence, Professor Begum Tokay





Faris Elasha (Cohort 5) School of Mechanical, Electrical

#### Low pressure, low cost hydrogen storage technology

Currently green hydrogen production and storage is focused primarily around electrolyser technology with high pressure storage. However, there are many uses for hydrogen aside from the transportation industry that do not require compressing hydrogen to high pressures. For example, in the context of adding Hydrogen to the gas supply system of up to 20 %, pressures to domestic premises can be between 75 mbar and 2 bar, a big step down from the 350-700 bar of a high pressure system. It makes more sense from an energy perspective to store the hydrogen at low pressures and avoid the round trip energy cost and the financial cost of the compressors and tanks. There is no low-pressure low-cost, hydrogen storage products on the market. Faris' research aims to understand the fundamental science behind low pressure hydrogen storage and design low pressure hydrogen storage systems using sustainability principles. Faris will also validate the technology and analyse the suitability and durability of the system using a small-scale test rig.

Supervisors: Dr Edward Barbour, Dr Jonathan Wilson





#### H2COOL - dual energy store for refrigerated transportation

Elizabeth's project will be part of H2COOL, a project which aims to develop metal hydrides to take advantage of their endothermic dehydrogenation, to provide cooling for refrigeration, in addition to hydrogen storage. This dual-use store has the potential application for transporting perishable goods in heavy goods vehicles, as the hydrogen release can be used for powering a hydrogen fuel cell whilst the cooling effect refrigerates the cargo space inside.

Supervisors: Professor David Grant, Assistant Professor Alastair Stuart, Dr Matthew Wadge, Professor Martin Dornheim







Amelia-Rose Edgley (Cohort 4) Faculty of Engineering



#### Nanostructured hydrogen storage materials for offshore green hydrogen

Metal hydrides are a more compact storage medium than compressed gas or liquid hydrogen. If a successful candidate can be found, metal hydrides can be used to simplify the equipment needed for an offshore hydrogen generation platform. Amelia is researching into higher capacity metal hydrides that are also resistant to the impurities found by generating hydrogen from seawater electrolysis.

Supervisors: Professor David Grant, Dr Marcus Adams





Joseph Parkinson (Cohort 5) School of Chemical Engineering



#### Novel materials and methods in electrocatalysis

Transition metal dichalcogenides (TMDs, e.g. MoS2, WS2) have been the subject of intense research in recent years as low-cost catalysts for the Hydrogen and Oxygen evolution reactions. The chemistry of the catalytically active sites is currently becoming more understood, and Joe's project seeks to build on these recent advances through:

- (i) Maximising edge sites through controlled TMD electrodeposition forming porous structures,
- (ii) Modifying the catalytic sites through metal doping,
- (iii) Optimising the stability of active sites,
- (iv) Elucidation of mechanistic detail

Supervisors: Dr Neil Rees, Dr Shangfeng Du

#### Sustainable Hydrogen Centre for Doctoral Training







Una O'Hara (Cohort 2) School of Chemistry



Figure: Raman equipment, University of Birmingham

#### **Development of high-performance complex hydrides**

Una is investigating thermodynamic tuning of boron and nitrogen-based complex metal hydrides (CMHs), synthesized by chemical and mechanochemical routes.

Nano-structuring by encapsulation in mesoporous-frameworks seeks to enhance cyclic stability, discharge and recharge rates whilst maintaining storage capacity. The materials will be characterised using a wide range of techniques to assess electrical, thermal and hydrogen storage properties.

Supervisors: Associate Professor Josh Makepeace, Professor David Book





Salim Ubale (Cohort 3) Faculty of Engineering



Stakeholder collaboration



#### Optimisation of PEM electrolyser balance of plant operation and maintenance to maximise performance and resilience of key infrastructure

Salim's project seeks to develop an asset management strategy for a hydrogen plant. Given the reliability issues faced by PEM electrolysers, the project aims to increase the reliability of the plant, thereby increasing its performance and to optimise the plant operation through the application of reliability and resilience engineering principles.

Supervisors: Dr Rasa Remenyte-Prescott, Professor David Grant, Assistant Professor Alastair Stuart







Shiqi Cui (Cohort 5) Belfast School of Architecture and the Built Environment (BSABE)



#### Safety of hydrogen and natural gas blends

Shiqi's research will focus on injecting hydrogen into natural gas pipelines and quickly mixing hydrogen and methane evenly. The homogeneous mixing of hydrogen and methane helps to prevent hydrogen embrittlement in the pipeline to prevent leakage from spreading. Safe handling of hydrogen and hydrogen-natural gas mixtures and understanding of the hazards and associated risks from leakage will also be included in future studies. These include (but are not limited to) hazard distances defined by the extent of the flammable cloud, and thermal effects from jet fire. Shiqi will focus on theoretical modelling and computational fluid dynamics (CFD) simulations. The research objective is to develop safety engineering tools related to hydrogen-methane mixtures and the effect of buoyancy on release.

Supervisors: Dr Sile Brennan, Dr Dmitriy Makarov, Professor Vladimir Molkov



#### Modular additive manufacturing for next-generation hydrogen storage

Compact hydrogen storage is a major challenge for hydrogen powered vehicles, with current state-of-the-art storage vessels being too large and operating at dangerously high pressures. Solid state Metal Hydrides (MH) can store large (relative to gaseous storage) quantities of hydrogen in much smaller volumes and at lower pressures, however current suitable candidate metals that reversibly store hydrogen are characterised by poor thermal conductivities which is detrimental to refuelling rates.

To improve heat transfer into the powdered metal, Yassin's PhD research aims to exploit the benefits and design freedom that Additive Manufacturing (AM) offers, by incorporating lattice structures into the vessel's internal architecture. This project will involve cell selection, lattice generation, mechanical design, numerical analysis, and experimental validation.

Supervisors: Dr Ian Maskery, Assistant Professor Alastair Stuart.







#### William Baker (Cohort 5) Faculty of Engineering



#### Sustainable hydrogen for agriculture and rural environments

William's project identifies and analyses the key factors that determine how distributed sustainable hydrogen generation can help decarbonize agriculture and bring the rural environment into the hydrogen economy. The rapidly changing global environment means that the work seeks to understand the impact of different factors, so that specific scenarios can be analysed, making the understanding gained widely applicable. An important part of the work is direct engagement with stakeholders to understand their priorities and undertaking fieldwork within the UK and USA to gain understanding differences of industrial and small-scale farming, to present real-world case studies.

Supervisors: Associate Professor Katy Voisey, Professor Jon Mckechnie



#### Highly efficient molecular hydrogen-evolution catalysts

Molecular hydrogen evolution electrocatalysts allow efficient hydrogen production from water under mild conditions.

Adedayo will research development of fully tailorable molecular clusters based on molybdenum/tungsten and sulfur/oxygen. Systems will be combined with conductive nanocarbon materials to develop highly efficient composite electrocatalysts for the water splitting reaction. The stability and efficiency of these systems will be explored during prolonged electrolysis.

We are looking to design a new generation of inexpensive electrocatalysts which could outperform state-of-the-art materials, while allowing atomic control of catalyst structure. The cheap and easy-to-prepare systems are particularly interesting from a commercialisation perspective, given the ease with which their preparation could be scaled-up.

Supervisors: Dr Graham Newton, Associate Professor Lee Johnson, Dr Kieran Jones







Chisom Okeke (Cohort 5) School of Mechanical, Electrical and Manufacturing Engineering



#### Low cost hydrogen technology for developing countries

Chisom's project aims to increase access to electricity and clean fuel by looking at the feasibility of a flow battolyser in underserved rural areas in Africa. The project will assess the use of a battolyser as a source of green hydrogen for cooking in conjunction with a solar panel based microgrid. This will require:

- Knowledge of hydrogen appliances and their uses in developing countries
- Understanding of economics behind the use of hydrogen
- Development of low cost appliances e.g. cooking and prototyping
- Testing and validation of low cost hydrogen appliance.

Supervisors: Dr Richard Blanchard, Dr Jonathan Wilson, Professor Dani Strickland



## Insights on metal nanoclusters (MNCs) (de)hydrogenation for on-board hydrogen storage application using electron microscopy and spectroscopy techniques

Ammonia is a rich source of hydrogen (17.8 wt%) and is suitable for room temperature and low-pressure storage. The use of catalysts addresses some of the challenges of ammonia decomposition, however the benchmark, ruthenium, poses scale up issues due to its cost. Thomas' project will explore bimetallic nanoclusters (diameters >2 nm), which are fundamentally different to metal nanoparticles where most metal atoms remain 'hidden' within the lattice, to present a potential solution, offering tuneable characteristics from more than one metal without the reliance on costly ruthenium. Advancing the viability of ammonia as a storage medium.

Supervisors: Associate Professor Jesum Alves Fernandes, Professor David Grant.







Samuel Balmer (Cohort 5) School of Chemistry



#### Supported nanoalloys for sustainable hydrogen production

Sam is researching supported nanoalloys for sustainable hydrogen production through photocatalysis. Sam's project aims to investigate the mechanisms that affect photocatalyst performance through pre- and post-reaction analysis using novel approaches to in-situ analysis.

Supervisors: Assistant Professor Anabel Lanterna, Associate Professor Jesum Alves Fernandes



#### Low-Coordinate 3d Metal Complexes as Alternatives to Platinum

Group Metals for Hydrogen Evolution Reaction

Rafael's project will develop a range of cobalt(I) organometallic complexes as single metal HER catalysts, where the metal centre is stabilised using highly sterically encumbering ligands. These unique complexes have never been investigated for HER chemistry, despite their favourable redox chemistry and substrate binding environment. The cobalt(I) compounds will be investigated for their redox chemistry and sensitivity to acid, along with their electrochemical response in the HER conditions.

Supervisors: Professor Deborah Kays, Associate Professor Graham Newton





Loughborough University

Redwan Atwiri (Cohort 5) Department of Aeronautical and Automotive Engineering



#### Reliability modelling of equipment engaged in the production (electrolysers) and usage of hydrogen

Redwan's project aims to improve the reliability and reduce the wear and tear of hydrogen production and consumption equipment, notably electrolysers. It addresses the current research gap in system and cell-level reliability of green hydrogen technology equipment. By using advanced reliability analysis techniques, the project will develop comprehensive models for equipment reliability and degradation. The methodology combines deterministic physics-based models, stochastic coloured petri nets, and machine learning to predict equipment lifespan. Validation will occur through experimental testing and system-level analysis, using shared data and literature. Redwan also plans to develop new methods to accelerate equipment degradation for more accurate reliability assessments.

Supervisors: Professor Lisa Jackson, Dr Ashley Fly





Samir Soares (Cohort 2) Faculty of Engineering



#### Hydrogen for a sustainable rural built environment

Samir is working to evaluate and model rural domestic energy systems and looking towards the opportunities and technologies to transition to low carbon energy consumption including technologies such as hydrogen fuel cells and boilers, with key considerations to energy accessibility challenges rural energy users face. Samir is also working on development of a green solid state hydrogen store with a digital twin.

Supervisors: Professor Mark Gillott, Assistant Professor Alastair Stuart









Efficient hydrogen separation using proton-conducting ceramic membranes and electrochemical cells

Most hydrogen used today is produced from fossil fuels (e.g., through steam reforming of natural gas, coal gasification). Product gases consist mainly of H2 and CO2, and other impurity gases (CH4 and CO). Energy-efficient and low-cost hydrogen separation constitutes a crucial process to move towards a hydrogen economy.Luke's project aims to achieve energy-efficient and low-cost hydrogen separation using proton conducting ceramic membranes for hydrogen rich streams, generated through reforming of natural gas as well as onsite purification of hydrogen close to the point of end use for dilute hydrogen streams; distributed through natural gas pipelines using ceramic proton electrochemical cells (hydrogen pumps). Dense ceramic membranes made of mixed protonic-electronic conductors (MPECs) are capable of separating hydrogen from gas mixtures with 100 % selectivity, reduced energy penalty and cost compared to well-established techniques such as pressure swing adsorption technique.

Supervisors: Dr Ming Li, Professor Begum Tokay, Professor David Grant.



#### Base metal catalysis of acceptorless alcohol dehydrogenation for hydrogen storage

Catalytic acceptorless alcohol dehydrogenation is an atom-economical approach for alcohol oxidation, without need for an oxidant. Reversible dehydrogenation/hydrogenation catalysis from this reaction provides a route to the use of organic molecules derived from biomass as liquid organic hydrogen carriers (LOHCs). Alcohols such as ethylene glycol, glycerol and the C4–C6 analogues erythritol, xylitol and sorbitol are considered to be potentially useful biomass-derived feedstocks; derived from agricultural or lumber resources, including waste streams and gravimetric hydrogen storage capacities, meeting targets set by the EU and the US Department of Energy. This chemistry has long been dominated by the platinum group metals (PGMs); however, low PGMs abundance means high economic and environmental cost, and their high toxicity means their removal from products can produce significant waste streams. Researchers are looking to other catalysts for industrial processes; with obvious candidates being base metals exhibiting low cost, high natural abundance, uniform global distribution and low toxicity. Isabelle's project will investigate a range of low coordinate and pincer complexes of the first-row transition metals in order to achieve the acceptorless dehydrogenation reactions and, with appropriate candidates, investigate the possibility of undertaking the reverse reaction with addition of H2.

Supervisors: Professor Deborah Kays, Professor Peter Licence.









Andreas loannides (Cohort 5) Faculty of Engineering



Figure 16 CO2 emissions per passenger for hydrogen against jet A fuel using seating arrangemer from 150-180 seats.

#### Assessing the environmental and economic sustainability of hydrogen and sustainable fuels for aviation

To achieve significant climate change mitigation in aviation, transitioning to low life cycle greenhouse gas (GHG) emission fuels is crucial. Sustainable aviation fuels (SAF), specifically drop-in fuels, offer near-term solutions by displacing conventional fuels without requiring modifications to existing infrastructure or aircraft engines. Hydrogen, a vital input for SAF production, plays a key role in various pathways. In the long term, direct use of hydrogen as an aviation fuel shows promise due to its higher energy density than conventional fuels, potentially improving aircraft fuel efficiency. However, adopting hydrogen fuels necessitates substantial changes in both aircraft technologies and ground systems. Andreas' project aims to comprehensively assess the potential of SAF and hydrogen fuels for low carbon aviation, considering technology readiness, fuel availability, techno-economic performance, and life cycle GHG and environmental implications.

Supervisors: Dr Ioanna Demetriou, Dr Vilius Portapas, Professor Jon McKenchnie



#### **Composite membranes for H2 purification**

H2 is a high quality and clean energy carrier. Most hydrogen is produced by steam methane reforming, followed by water-gas shift reaction, with biohydrogen production increasing. Before hydrogen is used in fuel cell and other applications CO2 and CH4 resulting from production processes has to be removed. Membrane-based separation technologies are promising alternatives to conventional separation technologies, i.e. pressure swing adsorption, due to low energy consumption. Many inorganic membranes of zeolites, metal alloys and carbon molecular sieves have been developed but scaling-up difficulties limit applications. Polymer membranes are useful, whilst controlling permeability/selectivity in harsh conditions is challenging. Recently, mixed matrix membranes (MMMs) – where inorganic material is embedded into polymer matrix – have attracted attention; as they combine porous materials' functionality with polymer processability. In this context, metal–organic frameworks (MOFs), comprised of metal ions connected by organic linkers, are most promising; due to their diverse and flexible structure. In addition, MOFs' organic linker typically have greater affinity towards polymer chains; allowing control of the MOF/polymer interface. Void-free MMMs can be prepared without requirement for modification of filler or membrane surfaces. Niko's project will explore development of MOF/polymer MMMs with enhanced H2 selectivity, to enable membrane based H2 purification.

Supervisors: Professor Begum Tokay, Assistant Professor Andrea Laybourn.







James Turner (Cohort 5) School of Chemistry



#### Modelling of photochemical water splitting based on charge accumulation in macrocycles

Photochemical water splitting using homogeneous catalysts provides a conceptually simple and promising route towards sustainable hydrogen production. At the heart of this processes lies a molecular photosensitizer along with a catalyst. Whereas such photoredox catalytic systems are well-established in other areas of synthetic chemistry, it is a particular challenge that photocatalytic water splitting requires a multielectron process where several electrons are accumulated in one molecular unit. These molecular systems that can accumulate several charges is provided by a class of recently developed macrocycles based on paracyclophanetetraene (PCT), where multiple charges can be stabilized with the occurrence of global aromaticity in the macrocycle. James will investigate prototype macrocyclic catalysts, contrast their properties with existing photoredox catalysts and suggest new candidates, through detailed computational studies.

Supervisors: Dr Felix Plasser, Dr Pooja Goddard



#### Innovative materials for thermal compression – Solving the challenge of hydrogen compression

Ramas' project focuses on overcoming challenges currently present in the field of hydrogen compression. Through utilizing the thermodynamics of metal hydrides, solid–state compression circumvents some of the economic and safety concerns present in mechanical compression. MHHC utilize high-pressure alloys to absorb hydrogen and compress it by heating the metal hydride. Ramas' project is centred around researching and developing suitable AB2 group alloys that will provide the desired isotherms with low hysteresis, flat pressure plateaus, and fast kinetics. Ramas aims to improve the efficiency of hydrogen compression through analysing hydrogen uptake, as well as thermodynamic and kinetic measurements for various alloy compositions. High-pressure alloy properties will be characterized by using analytical techniques such as XRD, SEM, and XPS. Moreover, Ramas' project also aims to evaluate and modify the design of existing solid-state compressor prototypes to enable its successful deployment for hydrogen compression applications.

Supervisors: Professor David Grant, Assistant Professor Alastair Stuart, Dr Marcus Adams







Mossen Randeree (Cohort 5) Department of Marketing

#### Developing a roadmap for adoption of sustainable hydrogen: A Delphi study of business and industry

Mossen's research aims to identify the challenges, barriers and opportunities for businesses involved in the transition to a low-carbon and sustainable hydrogen economy. Utilising a mixed method forecasting approach, including Delphi, Mossen will survey practitioners in a sector or industry and through interviews with experts and practitioners, the Delphi method will produce a clear road map for the adoption of hydrogen technologies that can inform policy, design and use.

Supervisors: Associate Professor Robert Cluley, Professor William Green





Gagan Krishna Gopakumar Suja (Cohort 5) Faculty of Engineering

#### Experimental study of renewable fuels for clean heavy-duty diesel engines

Renewable fuels are promising solutions to replace conventional fossil fuels across heavy transportation, as they are relatively clean (both at the production stage as well as in end use). Gagan's research will study one pathway for introducing renewable fuel into an existing heavy duty diesel engine. The experiments will involve using a much smaller amount of diesel to initiate power generation from the main renewable fuel, which will be injected into the engine separately of the diesel. Such an engine will still be capable of operating effectively on conventional diesel when renewable fuels are not available. Gagan's project aims to understand the detailed thermodynamics involved and to measure the efficiency and detailed emissions of the engine under a wide variety of operating conditions.

Supervisors: Professor Alastair Cairns, Professor Antonino La Rocca



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Loughborough	Odor additives for H <sub>2</sub>	$\frown$
Harvey Monroe (Cohort 2)	<ul> <li>Rationale design</li> <li>Chemical synthesis</li> <li>Benchmarking</li> </ul>	Rapid H <sub>2</sub> gas detection
Department of Chemistry	Leading to Improved H <sub>2</sub> safety	Odor agent

#### Development of odour additives for use in hydrogen technology

The remit of Harvey's project involves the design, synthesis and testing of novel compounds for use in hydrogen storage. A number of potential odorants will be selected and compared with the novel compounds, as well as some odorants present in literature.

The tests will consist of hedonic tone and odour character tests, to ensure the suitability of an odorant's scent before fuel cell tests are performed to test which odorants don't poison the catalyst. So far, work on the novel compounds has been fully focused on the bicyclopentane framework, due to its volatility and broad substrate scope.

Supervisors: Dr Marc Kimber, Dr Gareth Pritchard.



## Experimental study of advanced ammonia-fuelled, heavy duty, internal combustion (IC) engines under low load operation

Will is carrying out an experimental research project looking to utilise advanced combustion techniques such as turbulent jet ignition and dual fuel operation to enable the use of ammonia as a fuel in heavy duty, internal combustion engines; with a specific focus on low load operation, during which the combustion is the most challenged.

The project will be formed of two main studies, a fundamental combustion study carried out using a bespoke optical constant volume combustion chamber to understand flame development in a laminar environment, as well as an applied engine study, converting a diesel heavy duty compression ignition engine to operate using ammonia and hydrogen.

Supervisors: Professor Alasdair Cairns, Professor Antonino La Rocca, Dr Richard Jefferson-Loveday.







Alexandra Brochoire (Cohort 4) School of Chemical Engineering



#### Proton exchange membrane water electrolysers with thin film nanostructured electrodes

The biggest challenge with current proton exchange membrane water electrolysers (PEMWE) is their poor power performance and durability; which is mainly caused by large mass transfer losses and degradation of the electrode structure, from the random electrode structure from catalyst nanoparticles. Alexandra's PhD project will seek to develop a new generation of catalyst electrodes from aligned IrO2- and metal oxide-based nanowires for PEMWE applications; taking advantage of the high stability of nanowires and the boosted mass transfer characteristics of the unique thin catalyst layers from nanowire arrays.

Project aims are substrate surface modification approach to increase surface activity, in-situ nanowire array growing process based on IrO2 and metal oxide materials, surface deposition technique of SrIrO3 on nanowire arrays, and electrode evaluation using half-cell and single cell test.

#### Supervisors: Dr Shanfeng Du, Dr Neil Rees.



#### Hydrogen enrichment of natural gas by thermo-catalytic decomposition of methane

The gas network currently supplies natural gas to consumers but could supply gases, such as hydrogen, in the future. Thermo-catalytic decomposition of methane allows enrichment of natural gas with hydrogen, a carbon-free fuel.

Mickella's research is focused on the development of this technology and the incorporation of wind energy. Her research looks at the use of iron oxide from a natural source as the catalyst for the thermo-catalytic methane decomposition process.

Supervisors: Dr James Reynolds, Professor Sandie Dann and Professor David Saal.







Atish Gawale (Cohort 4) Belfast School of Architecture and the Built Environment



#### Safety strategies and engineering solutions for hydrogen heavy-duty vehicles

Pursuit of a low carbon economy means practical implementation of zero-emission applications, including hydrogen-fuelled heavy-duty vehicles (HDV) such as buses and trucks. Hydrogen's use in public transport implies stringent bus design requirements. Industry and regulators' concerns over HDV design, considered critical for successful roll-out, include:

1. Development of HDV refuelling protocol comparable with modern fossil-fuel vehicles, without jeopardising onboard compressed hydrogen storage system (CHSS) safety.

2. Fire-resistance rating of current CHSS, which may lead to rupture in a fire with catastrophic consequences, i.e. blast wave, fireball and projectiles.

Atish's project will review 'old' and new HDV hazards of different designs and sectors (buses and trucks); identifying and analysing existing prevention and mitigation safety strategies, engineering solutions, knowledge gaps and technological bottlenecks in provision of HDV safety.

Supervisors: Dr Sergii Kashkarov, Dr Dmitriy Makarov, Professor Vladimir Molkov.



#### Advanced hydrogen sensing platform based on functionalised metal-organic frameworks

Developing efficient sensor materials with superior performance for selective, fast and sensitive hydrogen detection is essential for environmental protection and human health. Metal–organic frameworks (MOFs) – crystalline and porous solid materials constructed from metal nodes (metal ions or clusters) and functional organic ligands – are of interest for gas sensing for their large surface area, adjustable pore size, tunable functional sites and intriguing properties; such as electrical conductivity, magnetism, ferroelectricity, luminescence and chromism. However, selectivity, sensitivity and stability are still major challenges for MOFs–based sensors used in hydrogen detection.

Emily's project aims to fabricate novel multifunctional MOFs with improved sensitivity and stability for hydrogen detection. The rational design of these robust, multifunctional MOFs will be guided by computational predictions; after integrating metal nodes, functional ligands, and guest molecules with different properties, to achieve selective sensing of hydrogen over multiple cycles. Computational modelling delivered in collaboration with Nottingham's Computational Materials Group.

Supervisors: Assistant Professor Oluwafunmilola Ola, Professor Elena Besley.

#### Sustainable Hydrogen Centre for Doctoral Training







Kieran Heeley (Cohort 2) Chemical Engineering



## Algal biomass to hydrogen: A circular approach for green sustainable processing with enhanced efficiency and minimal waste

Kieran's project investigates hydrothermal conversion of algal biomass to hydrogen-rich gas, in a sustainable circular approach. It looks at optimising the catalyst, feedstock and operating conditions to increase the hydrogen yield; whilst maximising the nutrient recovery.

Supervisors: Professor Bushra Al-Duri, Dr Rafael Orozco, Professor Lynne Macaskie.



#### Computational modelling of Solid-State Hydrogen Storage Materials

Sam's project aims to understand the composition-structure-property correlations of solid-state hydrogen storage materials, through accurate density functional theory simulations of both existing and hypothetical materials.

The most promising candidate materials discovered from the computational simulations will be synthesised and characterised, and their hydrogen storage properties will be validated by experiments.

Supervisors: Associate Professor Sanliang Ling, Professor Martin Dornheim, Professor David Grant.

#### Sustainable Hydrogen Centre for Doctoral Training







Mina Kazemi (Cohort 2) Belfast School of Architecture and the Built Environment (BSABE)



#### Prevention and mitigation of accidents with hydrogen-powered vehicles in confined spaces

The scope of Mina's doctoral study includes the identification and prioritisation of relevant knowledge gaps, to develop innovative safety strategies to mitigate and prevent hydrogen-fuelled vehicles accidents in confined spaces. The first step is performing analytical and numerical studies to increase hydrogen-powered vehicles' safety, through improving TRRDs design; to prevent pressure peaking phenomenon and blow-off phenomenon, which would both lead to hydrogen deflagration or detonation and catastrophe in confined spaces.

Supervisors: Dr Sile Brennan, Dr Dmitriy Makarov, Professor Vladimir Molkov.





John Taverner (Cohort 5) Department of Chemical Engineering



#### Understanding the lifecycle carbon footprint and costs of sustainable hydrogen energy systems

John's project delves into comprehensive research on current hydrogen production methods. Focussing on sustainability, this project involves developing analytical models to assess the carbon footprint associated with various hydrogen production techniques. By analysing the entire lifecycle of hydrogen energy systems, from production to utilisation, John's project aims to provide invaluable insights into environmental impact and cost-effectiveness.

Supervisors: Professor Wen-Feng Lin, Professor Jin Xuan.

#### Sustainable Hydrogen Centre for Doctoral Training







#### Vinay Patel (Cohort 5) School of Chemical Engineering



## Algal biomass to hydrogen: a circular approach for sustainable hydrogen production via eco-friendly supercritical water technology

Vinay's project aims to enhance the process of production of hydrogen-rich gas, by gasification of microalgae in supercritical water (SCW) medium. In general, algal biomass contains 20-30% carbohydrate, 10-20% lipid, and 40-60% protein. The ratio of the algae's composition fractions influences the effect of catalysts (K2CO3 or NaOH) and gasification products. Vinay will investigate hydrothermal conversion of algal biomass to H2-rich gas in a catalytic continuous process of supercritical water gasification (SCWG). Selected strains of wet microalgae (MA) are grown by modern methods (in a photo-bioreactor boosted light delivery, developed at University of Birmingham) to provide algal biomass feedstock.

Supervisors: Professor Bushra Al-Duri, Dr Rafael Orozco



#### High-throughput cycling coupled X-ray photoelectron spectroscopy (XPS) of hydrogen storage materials

Chris's research looks into the application of X-ray photoelectron spectroscopy (XPS) to samples after reactions at elevated pressures.

Chris is designing a sample transfer device that enables rapid X-ray photoelectron spectroscopy (XPS) analysis of samples after reactions at elevated pressures. The device will soon be used to investigate various solid-state hydrogen storage materials, with a particular focus on their change in performance with increasing hydrogen cycles.

Supervisors: Associate Professor James O'Shea, Professor David Grant.







Stephen Marr (Cohort 2) Department of Chemistry Stakeholder collaboration





## Development of techniques and methods for sampling, calibration and testing of hydrogen purity for fuel cell vehicles

Measurement challenges for hydrogen fuel cells are preventing the overall sector from growing. Stephen's project is looking at ways of developing a cylinder passivation technology, which would provide temporal stability data for the 14 trace contaminants outlined in ISO (International Organization for Standardization) 14687-2.

Supervisors: Dr Ben Buckley, Professor Upul Wijayantha, Dr Paul Holland.





Alex McGrath (Cohort 2) Faculty of Engineering Stakeholder collaboration





#### Synthesis and characterisation of metal alloys for hydrogen storage and related applications

Alex's project aims to experimentally synthesise new metal alloys shortlisted by computational screening; and characterise their physical, chemical and structural nature along with their thermodynamic and kinetic properties, during hydrogenation and de-hydrogenation. Alex is investigating synthesising new metal alloy compositions which will have improved hydrogen storage properties, forming their hydrides and characterising their microstructures.

Supervisors: Professor David Grant, Associate Professor Sanliang Ling

#### Sustainable Hydrogen Centre for Doctoral Training







Katarina Pegg (Cohort 3) School of Chemical Engineering



#### The role of green hydrogen in the West Midlands Combined Authority local energy system

Green hydrogen production from weather dependent low carbon generation is an area of growth signposted in the UK Committee on Climate Change's 6th Carbon Budget (published December 2020); which provides UK Government Ministers with advice on the volume of greenhouse gases the UK can emit during the period 2033-2037.

Katarina's research will focus on the advantages and disadvantages of green hydrogen generation at a local level, specifically within the West Midlands Combined Authority area.

Supervisors: Dr Grant Wilson, Professor Bushra Al-Duri.



#### Hydrogenation of storage materials

Oliver is undertaking research into the use of Machine Learning Potentials (MLPs), models that use machine learning to approximate the potential energy surface; with particular focus on High-Definition Neural Networks (HDNNs). With sufficient training data, MLPs enable large-size and long time-scale, accurate molecular dynamics simulations, which are unattainable via conventional methods.

Oliver has used MLPs to simulate a variety of Magnesium-Hydrogen systems, including hydrogenation of magnesium clusters. Future simulations, with larger atom counts and time scales, will be used to gain insight into the process of hydrogenation and may inform the selection of improved hydrogen storage materials.

Supervisors: Associate Professor Sanliang Ling, Professor David Grant.







Adam McKinley (Cohort 1) Department of Chemical Engineering



## Catalyst development for low-cost, large-scale sustainable hydrogen production from water and seawater using renewable energy sources

Adam is looking at the oxygen evolution and hydrogen production, via water and seawater splitting, driven by renewable energy. He is interested in the production and utilisation of low-cost, highly efficient and highly selective catalysts for the process. Adam is currently investigating the performance of Ruthenium and Palladium (Ru and Pd) nanoparticle-based electrodes for the hydrogen evolution reaction at varying temperatures. He aims to explore the prospect of a bifunctional catalyst capable of efficient and consistent performance in both the hydrogen evolution reaction and oxygen evolution reaction (HER and OER).

Supervisors: Professor Wen-Feng Lin, Professor Jin Xuan, Dr Darren Walsh.





Jai-Ram Mistry (Cohort 1) Department of Chemistry



#### Photocatalytic covalent organic frameworks for hydrogen production and storage

Jai undertakes research into the use of covalent organic frameworks (COFs) for hydrogen production and storage, as opposed to the popular metal organic frameworks (MOF) alternative.

His project involves the synthesis of new molecules which can be functionalised onto the surface of COFs; creating photocatalytic and size-specific channels which will permit hydrogen production from water and selective ingress, storage and egress.

Supervisors: Dr Iain Wright, Dr Simon Kondrat.







Patrick Powell (Cohort 3) School of Metallurgy and Materials



#### The use of hydrogen as a processing gas to produce rare earth magnets

Hydrogen is used in the conventional production of sintered (rare earth) neodymium-iron-boron magnets and in the recycling of these materials. In recent years new methods to manufacture rare earth magnets based on a process called the Hydrogen Ductilisation Process have been found.

This process reduces the number of processing steps, reduces waste and could give a significant economic advantage to magnet manufacture. However, the process is far from optimised and the aim of Patrick's project will be to develop this process.

Supervisors: Professor Allan Walton, Dr Richard Sheridan, Professor David Book.





Mulako Mukelabai (Cohort 3) Centre for Renewable Energy Systems Technology Wolfson School of Mechanical, Electrical, and Manufacturing Engineering



#### Renewable hydrogen production to transition to clean cooking

Mulako's project aims to develop technical and business models, and processes which will enable hydrogen produced from renewable energy to be utilised for cooking.

Though this process is understood, the system needs not just the right technology but also development of the right business model, human capacity and social acceptance to bring about the transformation of traditional cooking practices.

Supervisors: Dr Richard Blanchard, Professor Upul Wijayantha, Dr Alastair Livesey









Jacob Prosser (Cohort 1) Faculty of Engineering

$\frac{\text{MBH}_4 + nN}{\text{Systematic approach}}$	$H_3 \leftrightarrow MBH_4($	(NH <sub>3</sub> ) <sub>n</sub>
M = Li, Na, K, Ca, Mg, Ni, Sc, V and mixed metals		J.
Transportation	Cracking	Purification
<del></del> B	NH, N-0	

#### High capacity single and mixed metal borohydrides ammoniates for hydrogen energy storage applications

Jacob is researching the synthesis and characterisation of single and mixed metal borohydrides ammoniates (MBA/MMBAs), to increase the hydrogen storage performance of these materials and elucidate the reaction mechanisms of the decomposition process.

He is assessing the influence of metal charge density, electronegativity, additional metal cations and the number of ammonia ligands on the hydrogen storage performance.

Supervisors: Professor David Grant.





Aryamman Sanyal (Cohort 3) Department of Engineering



#### Reactor design and performance optimisation for catalytic hydrogen production from methane

Aryamman's project aims to design, develop and test a hydrogen generation reactor suitable for advanced catalyst; demonstrating high H2 yield and efficient carbon separation.

Natural gas into hydrogen and graphite has the potential to be highly disruptive and could be of substantial value if the process can be scaled up to commercial quantities.

Supervisors: Professor Weeratunge Malalasekera, Professor Upul Wijayantha







Srinivas Sivaraman (Cohort 3) Belfast School of Architecture and the Built Environment (BSABE)



#### Safety of Using Ammonia in the Hydrogen Economy

Owing to characteristics such as high energy density and the experience of the use of ammonia in industries; its transportation around the globe offers practical, cost-effective means of storing and transporting large quantities of hydrogen. Using ammonia as a hydrogen carrier and in fuel applications calls for a reassessment of hazards and risks. Srinivas's project aims to develop safety strategies and engineering solutions for the handling of large quantities of ammonia, used as a hydrogen carrier during transport and storage onboard, and the use of relevant infrastructure. His project will analyse the hazards – including toxicity effects, existing prevention and mitigation safety strategies – and perform comprehensive quantitative risk assessment for safe utilisation of ammonia as hydrogen carrier.

Supervisors: Dr Dmitriy Makarov, Prof Vladimir Molkov, Dr Volodymyr Shentsov.





Jack Shacklock (Cohort 2) Department of Chemistry



#### Lowering the H2 cost in methane cracking technology by using solid carbon as an energy storage material

Jack's research is designed to investigate the systematic alteration of process conditions to obtain value-added solid carbon, specifically for energy storage whilst still maintaining a high yield of hydrogen. Initial studies have been conducted to improve the methane cracking process to increase yield and longevity. By-product carbon has separated in batch processes and been studied in electrochemical supercapacitors, demonstrating a high rate of performance compared to commercial carbon used for supercapacitor manufacturing. These results suggest lowering the cost of turquoise hydrogen, by finding applications for by-product carbon, is promising. Further studies are currently underway to separate by-product carbon in real-time operation (as opposed to batch process) and evaluate their performance in applications.

Supervisors: Dr Simon Kondrat, Prof Upul Wijayantha







#### Zak Waite (Cohort 2) Faculty of Engineering

Stakeholder collaboration





#### To a 100% hydrogen domestic boiler

Zak's project seeks to redesign the domestic boiler so that hydrogen can be used as a network fuel. At the moment because methane, which is currently used, burns quite differently from hydrogen our existing domestic boilers cannot utilise hydrogen gas.

Supervisors: Dr Donald Giddings, Professor David Grant, Professor Robin Irons



#### Investigating the economic value of nuclear-hydrogen

As the generation mix in energy systems is characterised by an increasing penetration of generation from renewable energy sources (RES) energy imbalances are becoming more prevalent and potentially more costly to mitigate in the absence of flexible and cost-effective forms of storage. Kate's project will consider nuclear power as a potential source of both power and flexibility and explore the role, costs and potential value of nuclear to the wider energy system in its transition to net-zero and beyond.

Kate will investigate how conversion of nuclear based electricity into hydrogen not only provides storage and balancing opportunities but may also increase the return to and value of nuclear investments, by providing alternative vectors for storing and consuming energy derived from nuclear power. Kate's research aims to develop a tool for assessing economic costs and benefits of nuclear power with hydrogen to the GB energy system.

Supervisors: Professor David Saal, Associate Professor Grant Wilson, Professor Monica Giulietti







Joseph Walton (Cohort 4) School of Chemical Engineering

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#### Business cases for green hydrogen

It is generally agreed that hydrogen employed in sustainable and emission-reducing projects needs to be sourced from 'green' feedstock and energy. Nevertheless, the vast majority of hydrogen sold today is 'black' and produced by steam reforming of natural gas. Obviously, there are cost issues. Joseph's work will look into how green hydrogen can be costed, so that it is more compatible with today's energy system. This will include analysing business cases, high-value applications, externalities and options to sell 'greened' products; based on green hydrogen application. Research aims to deliver cost model fully established, environmental pricing added to cost model, business model development concluded; and dialogue with industry, with validation of models and approaches.

Supervisor: Professor Robert Steinberger-Wilckens.



#### Manufacturing conductive oxides as catalyst support for energy efficient production of hydrogen and ammonia

Lukas will investigate a variety of solid oxides such as alumina and yttrium-stabilised zirconia and with the aim of characterising a number of properties such as their composition, crystal structures and conductivity, the end goal being to improve their performance in a number of roles such as catalyst supports, solid oxide electrolyser/fuel cell electrolytes, and membranes. This will involve creating and understanding new compositions of materials through doping and defect chemistry, in order to enhance processes such as hydrogen and ammonia production through increased efficiency and performance.

Supervisors: Dr Ming Li, Professor David Grant, Associate Professor Sanliang Ling



### **Student Publications as of October 2023**

SusHy Student	Publication
Adam McKinley	Layered double hydroxide-based electrocatalysts for the oxygen evolution reaction: identification and tailoring of active sites, and superaerophobic nanoarray electrode assembly. Chemical Society Reviews, 50(15), pp.8790-8817.
Edward Jones	Characterisation of ethylene adsorption on model skeletal cobalt catalysts by inelastic and quasi-elastic neutron scattering. Cataly- sis Communications, 163, p.106409.
Jai-Ram Mistry	Simultaneous enhancement of thermally activated delayed fluorescence and photoluminescence quantum yield via homoconjuga- tion. Journal of Materials Chemistry C, 10(16), pp.6306-6313.
sar nam misery	Homoconjugation effects in triptycene based organic optoelectronic materials. Materials Advances, 4(3), pp.787-803.
Mina Kazemi	Numerical modelling of sustained hydrogen combustion and flame blow-off from a TPRD. In Proceedings of the 10th International Seminar on Fire and Explosion Hazards (ISFEH10) (pp. Paper-ID63).
	Renewable hydrogen economy outlook in Africa. Renewable and Sustainable Energy Reviews, 167, p.112705.
	Hydrogen technology adoption analysis in Africa using a Doughnut-PESTLE hydrogen model (DPHM). International Journal of Hydro- gen Energy, 47(74), pp.31521-31540.
Mulako Dean Mukelabai	Hydrogen for Cooking: A Review of Cooking Technologies, Renewable Hydrogen Systems and Techno-Economics. Sustainability, 14 (24), p.16964.
	Using machine learning to expound energy poverty in the global south: Understanding and predicting access to cooking with clean energy. Energy and AI, 14, pp.100290.
Srinivas Sivaraman	Quantitative Risk Assessment Methodology for Hydrogen Tank Rupture in a Tunnel Fire. Hydrogen, 3(4), pp.512-530.
Mickella Dawkins	An iron ore-based catalyst for producing hydrogen and metallurgical carbon via catalytic methane pyrolysis for decarbonisation of the steel industry. International Journal of Hydrogen Energy, 48(57), pp.21765-21777.
Jack Shacklock	Superior Rate Capability of High Mass Loading Supercapacitors Fabricated with Carbon Recovered from Methane Cracking. Inorgan- ics, 11(8), p.316.
Kieran Heeley	Supercritical water gasification of microalgal biomass for hydrogen production-A review. International Journal of Hydrogen Energy, 49, Part A, pp 310-336
Hazhir Ebne-Abbasi	CFD Model of Refuelling through the Entire HRS Equipment: The Start-Up Phase Simulations. Hydrogen, 4(3), pp.585-598.



### **Selected Student Presentations**

SusHy Student	Presented their research at
Jacob Prosser, Chris Ryder, Alex McGrath, Oliver Morrison	17th International Symposium on Metal-Hydrogen Systems (MH2022)
Courtney Quinn	2022 Early Career Researcher Regional Symposium on Electrochemistry
Mina Kazemi, Hazhir Ebne- Abbasi, Srinivas Sivaraman	International Summer School in Hydrogen and Fuel Cells Technology and 10th International Conference on Hydrogen Safety
Kieran Heeley	14th International Solvothermal and Hydrothermal Association Conference
Patrick Powell	27th International Workshop on Rare Earth and Future Permanent Magnets and their Applications



## Some of our Highlights



Stakeholder workshop



Power Trader Workshop





Dayo at FMOCS VII



Paddy receiving a CDT conference reward



Fire and Explosion Hazard Conference



Cohort 4 induction week



Oliver presenting at CDT conference



Una doing outreach



Away day



Glastonbury outreach



CDT Conference



CDT conference posters





CENTRE FOR DOCTORAL TRAINING

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SusHy (Sustainable Hydrogen Centre for Doctoral Training) CDT



Sustainable Hydrogen Centre for Doctoral Training























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